Structure 1a

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   17 SEP 2002  HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES:  17 SEP 2002  HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his

     (FILE 'HCAPLUS' ENTERED AT 09:19:37 ON 19 SEP 2002)
               DEL HIS Y

     FILE 'REGISTRY' ENTERED AT 09:23:58 ON 19 SEP 2002

     FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002

=> d que stat
NO L# DEFINED

=> fil reg
FILE 'REGISTRY' ENTERED AT 09:24:21 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   17 SEP 2002  HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES:  17 SEP 2002  HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf
```
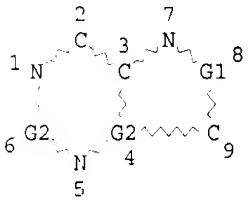
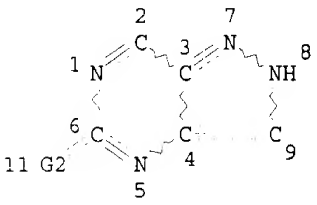

```
=> d his

     (FILE 'HCAPLUS' ENTERED AT 09:19:37 ON 19 SEP 2002)
               DEL HIS Y

     FILE 'REGISTRY' ENTERED AT 09:23:58 ON 19 SEP 2002

     FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002
               ACT ONEA/A
               ---------
L1             STR
L2   (      6184)SEA FILE=REGISTRY SSS FUL L1
L3             STR
L4           17 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
               ---------

     FILE 'REGISTRY' ENTERED AT 09:24:21 ON 19 SEP 2002

=> d que stat l4
L1             STR
```




```
VAR G1=C/N/O/S
VAR G2=C/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L2   (      6184)SEA FILE=REGISTRY SSS FUL L1
L3             STR
```



N~~N~~N
@12 13 14

Me~N~~Me
15 @16 17

S~~Me
@18 19

```
VAR G2=H/NH2/16/12/F/CN/OME/18/SH/OH/CL/NO2/CF3/ME/ET
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
```

NUMBER OF NODES IS 18

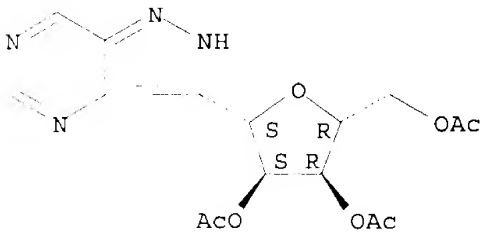
STEREO ATTRIBUTES: NONE
L4 17 SEA FILE=REGISTRY SUB=L2 SSS FUL L3

100.0% PROCESSED 3644 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

=> d l4 ide can 1-17

L4 ANSWER 1 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-72-6 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 2,3,5-triacetate, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H18 N4 O7
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

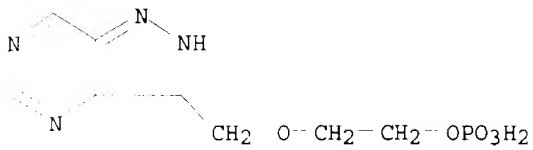


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-71-5 REGISTRY
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)
MF C8 H11 N4 O5 P . 2 Na
SR CA
LC STN Files: CA, CAPLUS

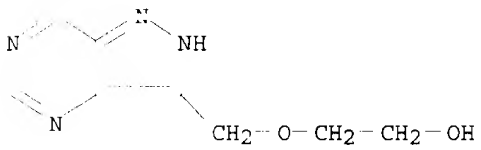


●2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-70-4 REGISTRY
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C8 H10 N4 O2
SR CA
LC STN Files: CA, CAPLUS



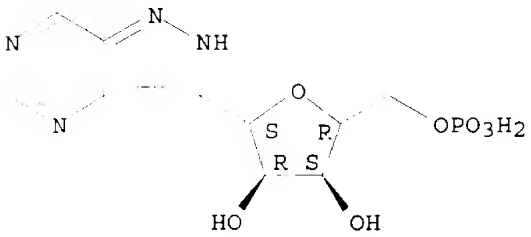
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 4 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-69-1 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 5-(dihydrogen phosphate), disodium salt (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H13 N4 O7 P . 2 Na
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



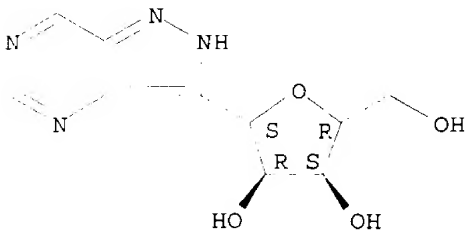
●2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 5 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-67-9 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H12 N4 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

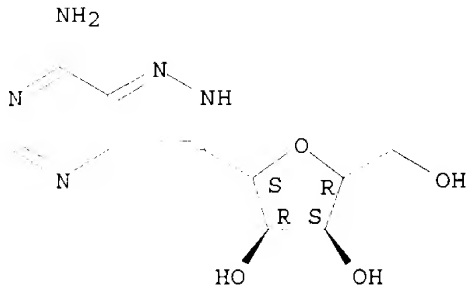
REFERENCE 1: 134:237749

REFERENCE 2: 133:222974

L4 ANSWER 6 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 123238-52-8 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, conjugate monoacid, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH

MF C10 H13 N5 O4 . H
SR CA
LC STN Files: CA, CAPLUS
CRN (57101-52-7)

Absolute stereochemistry.

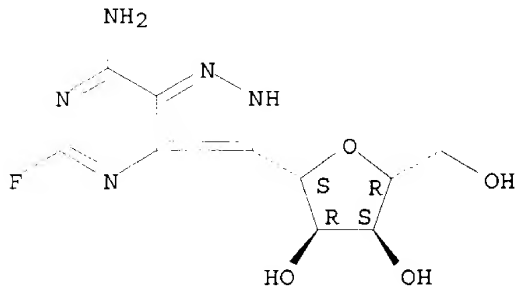


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

L4 ANSWER 7 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 123162-34-5 REGISTRY
CN D-Ribitol, 1-C-(7-amino-5-fluoro-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H12 F N5 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



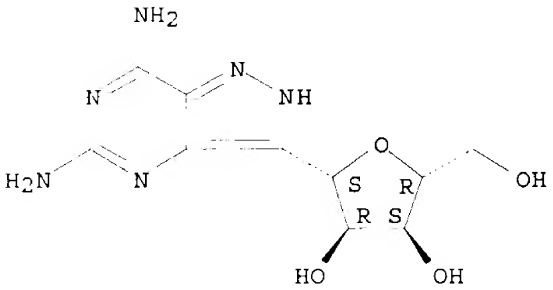
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

L4 ANSWER 8 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 123162-33-4 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-(5,7-diamino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H14 N6 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

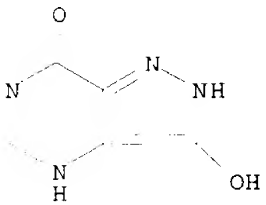


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

L4 ANSWER 9 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 87499-14-7 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-hydroxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C5 H4 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



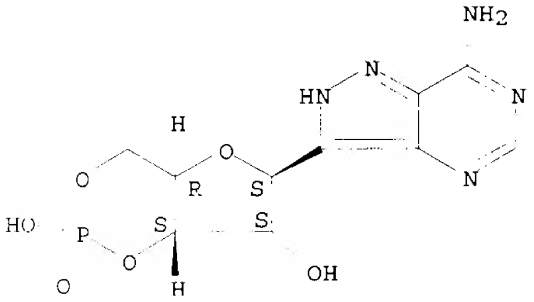
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:158362

L4 ANSWER 10 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 71972-01-5 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN 4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H12 N5 O6 P
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

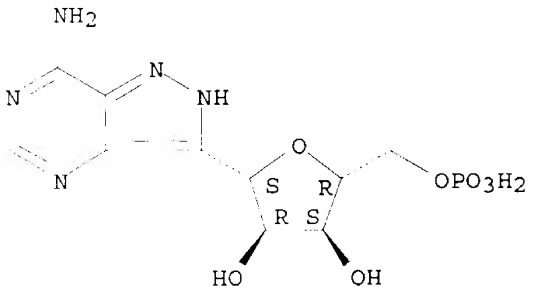


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 91:211773

L4 ANSWER 11 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 71972-00-4 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H14 N5 O7 P
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



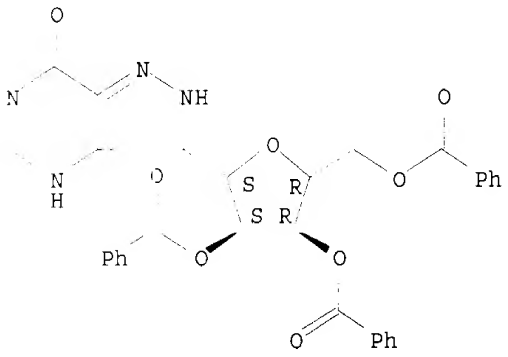
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 91:211773

L4 ANSWER 12 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 67560-82-1 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H24 N4 O8
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



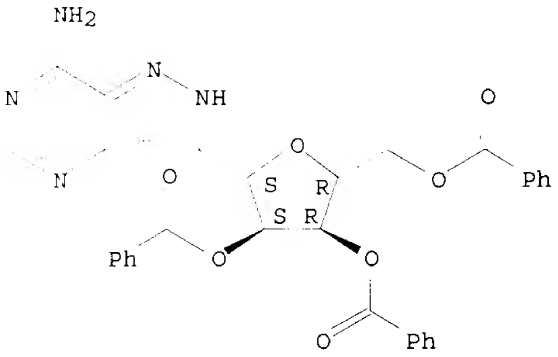
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:197857

L4 ANSWER 13 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 67560-80-9 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C31 H25 N5 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



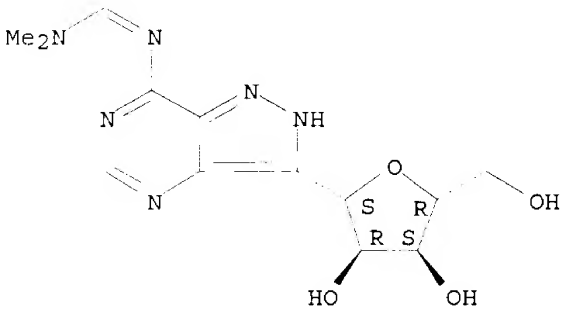
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:197857

L4 ANSWER 14 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 63358-78-1 REGISTRY
CN Methanimidamide, N,N-dimethyl-N'-(3-.beta.-D-ribofuranosyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, methanimidamide deriv.
FS STEREOSEARCH
MF C13 H18 N6 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

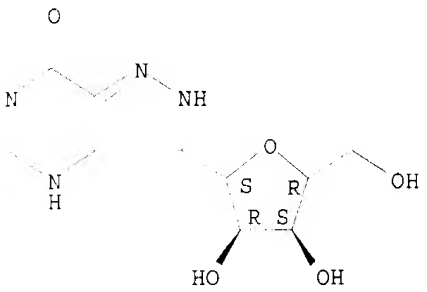
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:68560

L4 ANSWER 15 OF 17 REGISTRY COPYRIGHT 2002 ACS

RN 63347-44-4 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H12 N4 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



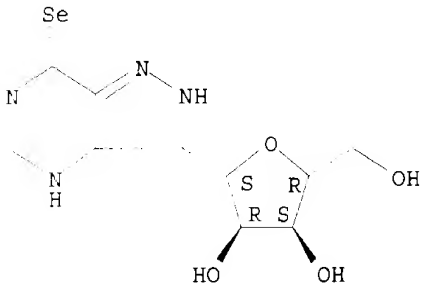
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:68560

L4 ANSWER 16 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 57101-53-8 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidine-7-selone, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H12 N4 O4 Se
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



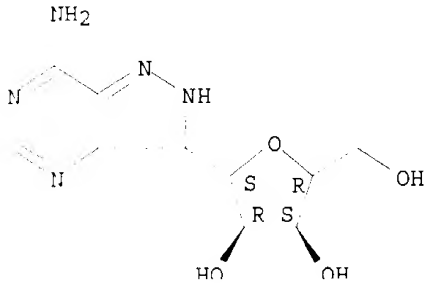
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:97797

L4 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 57101-52-7 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
OTHER NAMES:
CN 2H-Formycin
FS STEREOSEARCH
MF C10 H13 N5 O4
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1967 TO DATE)
7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 121:83847

REFERENCE 2: 112:212992

REFERENCE 3: 111:166765

REFERENCE 4: 93:113653

REFERENCE 5: 89:110233

REFERENCE 6: 87:68560

REFERENCE 7: 83:97797

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:24:41 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 19 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 18 Sep 2002 (20020918/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> s l4
L5 12 L4

=> d .ca hitstr l5 1-12]
'1-12]' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
ENTER DISPLAY FORMAT (BIB):end

=> d .ca hitstr l5 1-12

L5 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:139773 HCAPLUS
DOCUMENT NUMBER: 134:237749
TITLE: Design and Synthesis of Inhibitors of Adenosine and AMP Deaminases
AUTHOR(S): Bojack, Guido; Earnshaw, Christopher G.; Klein, Robert; Lindell, Stephen D.; Lowinski, Christian; Preuss, Rainer
CORPORATE SOURCE: Aventis CropScience GmbH, Frankfurt am Main, D-65926, Germany
SOURCE: Organic Letters (2001), 3(6), 839-842
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nucleosides and nucleotides which are able to undergo covalent hydration in the aglycon ring system are potential inhibitors of the enzymes adenosine deaminase (ADA) and AMP deaminase, resp. Calcns. of the enthalpy of covalent hydration and of enzyme binding energy have been used to design new inhibitors of ADA. The ribosyl triazolotriazine I, which was synthesized as a result of these calcns., exists predominantly as the covalent hydrate II in water and is a potent inhibitor of mammalian ADA (IC50 50 nM). In addn., biol. testing of the I/II mixt. showed that it possessed postemergence herbicidal activity at rates of 320 g ha-1 and below, depending upon the species.
CC 33-9 (Carbohydrates)
Section cross-reference(s): 5, 7
IT 550-33-4, Nebularine 13264-01-2, Deaminoformycin 206450-52-4
254114-35-7 254440-94-3 **291536-67-9** 330469-91-5
330469-92-6

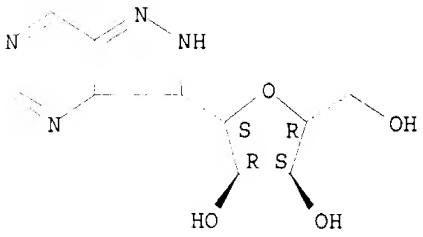
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

IT **291536-67-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

RN 291536-67-9 HCAPLUS

CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:665549 HCAPLUS
DOCUMENT NUMBER: 133:222974
TITLE: Preparation of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine
INVENTOR(S): Bojack, Guido; Lindell, Stephen; Rosinger, Christopher; Dudfield, Philip; Earnshaw, Christopher
PATENT ASSIGNEE(S): Aventis Cropscience Gmbh, Germany
SOURCE: Ger. Offen., 82 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19912636	A1	20000921	DE 1999-19912636	19990320
WO 2000056734	A1	20000928	WO 2000-EP2206	20000313
W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1165563	A1	20020102	EP 2000-916932	20000313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: DE 1999-19912636 A 19990320
WO 2000-EP2206 W 20000313

OTHER SOURCE(S): MARPAT 133:222974

AB Title compds. [(I); Q = N, CR1; Q1 = C,N; if Q1 = C, bond Q1-C2 = double; if Q1 = N, bond C2-Q2 = double; Q2 = N, CR2, when Q1 = N, or NR2, O, S, S(O), SO2, when Q1 = C; R = (un)satd. hydrocarbon chain substituted with O, S, NHR4; R1, R2 independently = H, NHR3, OR3, SR3, CN, halogen, N3, NO2, SF5; R3 = H, acyl, (un)satd. (cyclo)alkyl, SO2NH2; R4 = alkyl], useful as herbicides, plant growth regulators, and for the treatment of disease as adenosine monophosphate deaminase or adenosine deaminase regulators, were prepd. Thus, in four steps, starting from 2',3',5'-tri-O-acetyl-8-aza-9-deaza-inosine, (II) was prepd. (isolated as the disodium salt). In in vitro adenosine monophosphate deaminase regulation tests in pea plants or calf intestine, II had .gtoreq. 50% inhibition of enzyme activity at 500.mu.M. Similar compds. were tested for activity with adenosine deaminase from rabbit muscle, and also proved active.

IC ICM C07H007-06
ICS C07H023-00; C07H009-04; C07H015-26; C07D487-04; C07D519-00; A01N043-90; A01N057-16; A01N055-10; A61K031-66; A61K031-695; A61K031-70

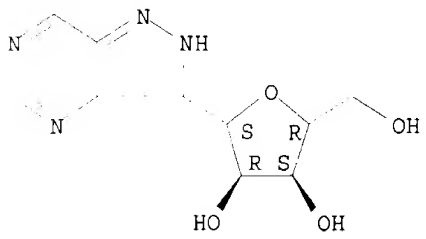
CC 33-9 (Carbohydrates)
Section cross-reference(s): 5, 28, 63

IT 244035-94-7P 254114-35-7P 254440-94-3P **291536-67-9P**
291536-68-0P **291536-69-1P 291536-70-4P**
291536-71-5P 291536-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

IT **291536-67-9P 291536-69-1P 291536-70-4P**
291536-71-5P 291536-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

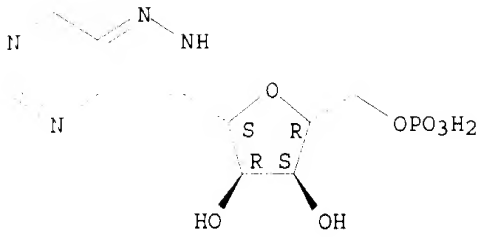
RN 291536-67-9 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



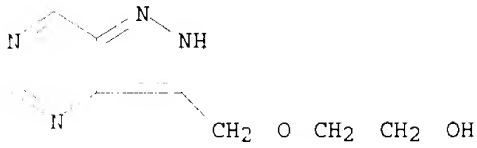
RN 291536-69-1 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 5-(dihydrogen phosphate), disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

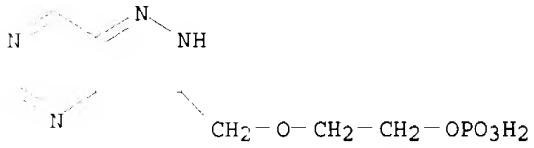


●2 Na

RN 291536-70-4 HCAPLUS
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)- (9CI) (CA INDEX NAME)



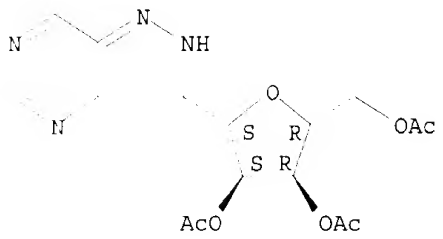
RN 291536-71-5 HCAPLUS
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)



●2 Na

RN 291536-72-6 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 2,3,5-triacetate, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

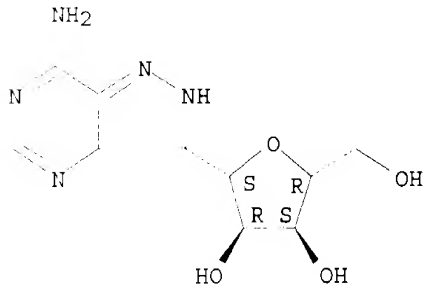


L5 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:483847 HCAPLUS
DOCUMENT NUMBER: 121:83847
TITLE: Tautomerism, protonation, and ionization of formycin in aqueous solution by the pH dependence of 13C chemical shifts and 13C-1H coupling constants
AUTHOR(S): Cho, Bongsup P.; McGregor, Michael A.
CORPORATE SOURCE: Coll. Pharm., Univ. Rhode Island, Kingston, RI, 02881, USA
SOURCE: Nucleosides & Nucleotides (1994), 13(1-3), 481-90
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Analyses of the pH dependence of 13C chem. shifts and 13C-1H coupling consts. of formycin in aq. soln. revealed two pKa's, at 4.4 and 9.7, corresponding to a protonation at N4 and an ionization at N1. The N4-protonation results in the transfer of a pyrazolo ring hydrogen from N1 to N2. At physiol. pH, formycin was found to exist as a mix. of N1H and N2H tautomers, with the former being predominant (>94%).

CC 33-9 (Carbohydrates)
Section cross-reference(s): 22
IT 6742-12-7 **57101-52-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(tautomerism, protonation, and ionization of, in aq. soln.)
IT **57101-52-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(tautomerism, protonation, and ionization of, in aq. soln.)
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

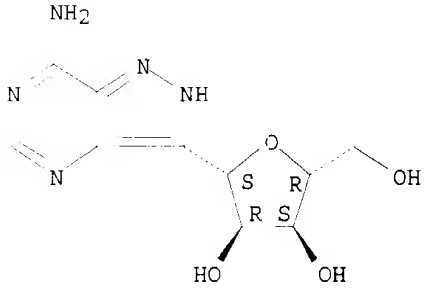


L5 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:212992 HCAPLUS
DOCUMENT NUMBER: 112:212992
TITLE: A quantum chemical study of the enzymic deamination of benzoadenine derivatives. A theoretical model of the interactions occurring between nucleosides and the active site of adenosine deaminase
AUTHOR(S): Orozco, Modesto; Canela, Enric I.; Franco, Rafael
CORPORATE SOURCE: Fac. Quim., Univ. Barcelona, Barcelona, E-08028, Spain
SOURCE: Eur. J. Biochem. (1990), 188(1), 155-63
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A theor. study is presented, where, by using both ab initio and semi-empirical methodologies, the properties of benzoadenine derivs. as substrates of adenosine deaminase are discussed. The results suggest that lin-benzoadenine and lin-benzoadenosine can be recognized with an affinity similar to that of adenosine, but only if they are introduced about 0.12 nm deeper inside the active site of the enzyme than the natural substrate adenosine. This fact implies the existence of nonlinear H bonds inside the active site of adenosine deaminase. Ab initio mol. electrostatic potential values suggest that these H bonds can exist, and have stability similar to that of linear H bonds. Finally, the great rate of deamination of lin-benzoadenine, comparable with that of adenosine-despite the absence of the ribose, is explained in the context of the hypothesis that the protonation at the N1 atom is the rate-detg. step of the whole deamination reaction.

CC 7-4 (Enzymes)
IT 58-61-7 Adenosine, reactions 69-33-0 73-24-5, Adenine, reactions 6736-58-9, 3-Deazaadenosine 6742-12-7 14432-09-8, 1-Deazaadenosine 53449-12-0, lin-Benzoadenine 53449-43-7, Prox-benzoadenine 53449-44-8, Dist-benzoadenine **57101-52-7** 60189-62-0, Lin-Benzoadenosine 60189-88-0 90108-76-2, 1H-Benzimidazo[5,6-g]quinazolin-9-amine 115420-04-7, 4,9-Dihydro-lin-benzoadenine
RL: RCT (Reactant)
(reaction of, with adenosine deaminase, quantum chem. study of)
IT **57101-52-7**
RL: RCT (Reactant)
(reaction of, with adenosine deaminase, quantum chem. study of)
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:566765 HCAPLUS
DOCUMENT NUMBER: 111:166765
TITLE: Theoretical study of the tautomerism of adenosine and formycin: functional implications
AUTHOR(S): Orozco, M.; Canela, E. I.; Lluis, C.; Mallol, J.; Franco, R.
CORPORATE SOURCE: Fac. Quim., Univ. Barcelona, Barcelona, 08028, Spain
SOURCE: Prog. Clin. Biol. Res. (1989), 291(QSAR: Quant. Struct.-Act. Relat. Drug Des.), 365-8
CODEN: PCBRD2; ISSN: 0361-7742
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The relative energies of amino-imino tautomers of adenosine and N7- and N8-H tautomers of formycin protonated at N1 were calcd. The amino form of adenosine and the N8-H form of formycin were more stable based on data obtained by MNDO, AM 1, and ab initio STO-3G methods. The tautomerism under various reaction conditions may influence nucleoside deamination by adenosine deaminase.

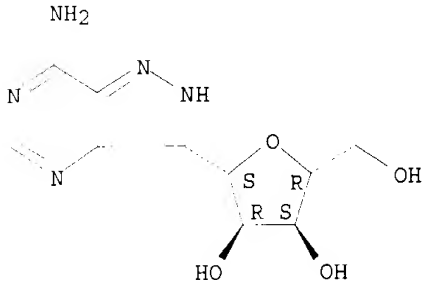
CC 1-3 (Pharmacology)

IT 58-61-7, Adenosine, biological studies 146-78-1, 2-Fluoroadenosine 2096-10-8, 2-Aminoadenosine 6742-12-7 **57101-52-7** 82538-40-7 **123162-33-4** **123162-34-5** 123179-97-5 **123238-52-8**
RL: PRP (Properties)
(relative energy of, tautomerism and metab. by adenosine deaminase in relation to)

IT **57101-52-7** **123162-33-4** **123162-34-5** **123238-52-8**
RL: PRP (Properties)
(relative energy of, tautomerism and metab. by adenosine deaminase in relation to)

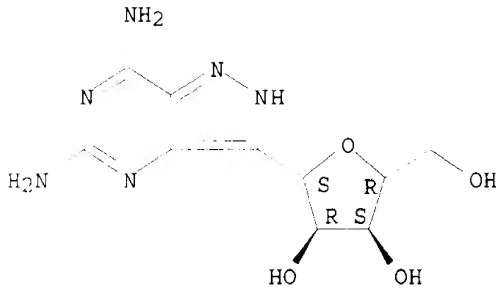
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



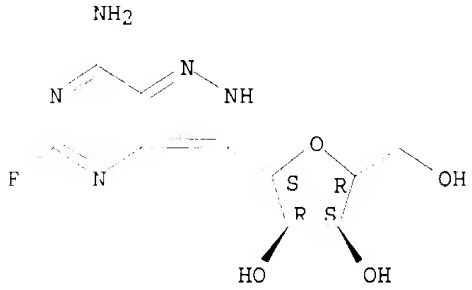
RN 123162-33-4 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-(5,7-diamino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



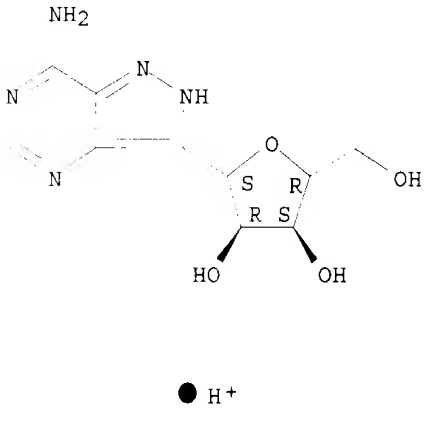
RN 123162-34-5 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-5-fluoro-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 123238-52-8 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, conjugate monoacid, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:558362 HCAPLUS
DOCUMENT NUMBER: 99:158362

TITLE: Synthesis of 2-substituted 2,6-dihydro-3-hydroxy-7H-pyrazolo[4,3-d]pyrimidin-7-ones
AUTHOR(S): Ochi, Hisao; Miyasaka, Tadashi
CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Tokyo, 142, Japan
SOURCE: Chem. Pharm. Bull. (1983), 31(4), 1228-34
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:158362

AB Pyrazolo[4,3-d]pyrimidines I (R = Ph, p-tolyl, m-tolyl, 4-ClC6H4) were prepd. by redn. of Et 4-nitrosopyrazole-3-carboxylates II (R1 = NO) and condensation of the resulting II (R1 = NH2) with HCONH2 . II (R = NO) were prepd. by nitrosating II (R1 = H), which were prepd. from EtO2CCOCH2CO2Et and RNHNH2.

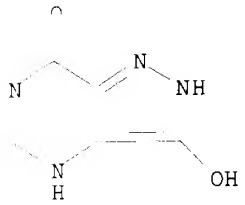
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **87499-14-7P** 87499-15-8P 87499-16-9P 87499-17-0P
87499-18-1P 87499-19-2P 87499-23-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **87499-14-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 87499-14-7 HCAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:513653 HCAPLUS
DOCUMENT NUMBER: 93:113653
TITLE: Tautomerism of formycin. Mechanism of interconversion
AUTHOR(S): Dodin, Guy; Bensaude, Olivier; Dubois, Jacques Emile
CORPORATE SOURCE: Inst. Topol., Univ. Paris, Paris, 75005, Fr.
SOURCE: J. Am. Chem. Soc. (1980), 102(11), 3897-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

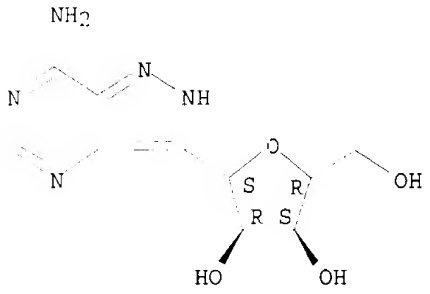
AB The tautomeric equil. between 1H- and 2H-formycin (7-amino-3.beta.-D-ribofuranosyl-1H-pyrazolo[4,3-d]pyrimidine) has a const. KT = N(2)H/N(1)H = 0.2 and an enthalpy estd. as 1 kcal mol-1. The tautomeric interconversion is catalyzed by H+ (kH+ = 3 .times. 109 M-1 s-1) and by OH-(kOH = 5 .times. 109 M-1 s-1). No other catalytic pathway such as water catalysis or tautomerization via tautomeric cations contributes significantly to the interconversion. Protonation of formycin does not occur significantly on the pyrazole ring.

CC 22-6 (Physical Organic Chemistry)

IT 6742-12-7 **57101-52-7**
RL: RCT (Reactant)
(tautomerization of, kinetics and thermodn. of)

IT **57101-52-7**
RL: RCT (Reactant)
(tautomerization of, kinetics and thermodn. of)
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



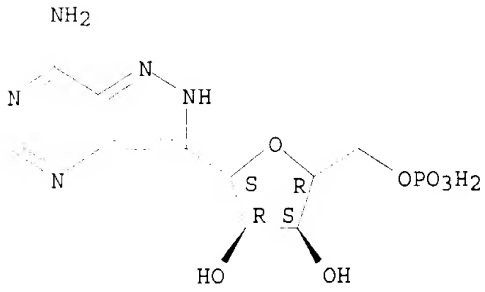
L5 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:611773 HCAPLUS
DOCUMENT NUMBER: 91:211773
TITLE: Formycin 3',5'-cyclic phosphate
INVENTOR(S): Umezawa, Sumio; Umezawa, Hamao; Kawamura, Kenji; Makabe, Osamu
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54088295	A2	19790713	JP 1977-154396	19771223
JP 61002072	B4	19860122		

AB A mixt. of 4.5 mL (MeO)3PO, 0.6 mL POCl3, and 1 g formcyin was stirred 2 h at -5.degree. and treated with Dowex 50W .times. 8 (H+) to give 845 mg formycin-5'-phosphate (I). Dicyclohexylcarbodiimide (1.65 g) in pyridine was added to a refluxing mixt. of 1.46 g I and 200 mL (Me2N)3PO in pyridine over 1 h, the whole refluxed 1 h, allowed to stand overnight at room temp., stirred with H2O at room temp., and treated with Dowex 50W .times. 8 (H+) to give 41% II (R = H). II (R = Me, Me2CH) were also prepd.
IC C07H007-06
CC 33-7 (Carbohydrates)
IT **71972-00-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
IT 67187-18-2P **71972-01-5P** 71972-02-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **71972-00-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)

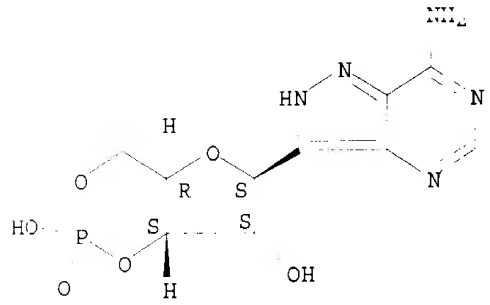
RN 71972-00-4 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **71972-01-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71972-01-5 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:597857 HCAPLUS
DOCUMENT NUMBER: 89:197857
TITLE: Synthesis of pyrazoles. A simple preparative synthesis of C-nucleosidic antibiotics formycin and formycin B
AUTHOR(S): Kalvoda, Ladislav
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, Czech.
SOURCE: Collect. Czech. Chem. Commun. (1978), 43(5), 1431-7
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Formycin (I, R1 = H) and formycin B (II, R1 = H) were synthesized by a route based on cycloaddn. of N2CHR2 to NCCR3:CHCO2R4 with elimination of HCN yielding pyrazoles III. Thus, 3,4,6-tri-O-benzoyl-2,5-anhydro-D-allonic acid was converted with SOCl2 to chloride and treated with Ph3P:CHCO2CMe3 in the presence of HCN to yield 60% tert-Bu

(Z)-3-cyano-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)propenoate, which was treated with N2CHCN or N2CHCO2Et to give, resp., 86% IV (R5 = CO2CMe3, R6 = CN) (V) and 73% IV (R5 = CO2CMe3, R6 = CO2Et) (VI). The CMe3 group of V was split off with HCO2H at 60-70.degree. and the acid was heated with NEt3, Cl3CCH2OH, and (PhO)2P(O)N3 in PhMe 5 h at 100.degree. to yield 36% IV (R5 = NHCO2CH2CCl3, R6 = CN). The CH2CCl3 group was cleaved with Zn dust and NH4Cl in boiling MeOH and the product was cyclized by heating with HN:CHNH2 to yield 29.5% I (R1 = Bz) (VII). Analogously, VI gave 58% IV (R5 = NHCO2CH2CCl3, R6 = CO2Et) which yielded 67% II (R1 = Bz) (VIII). Methanolysis of VII and VIII gave 90% formycin and 95% formycin B, identical with natural antibiotics prepd. by fermn.

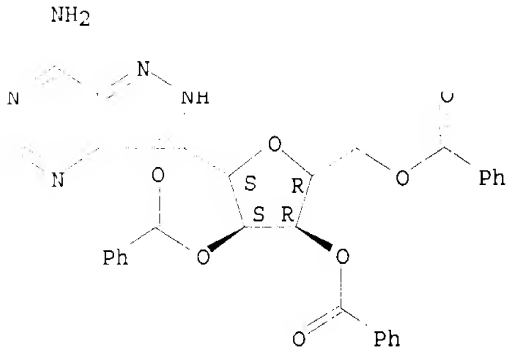
CC 33-7 (Carbohydrates)
Section cross-reference(s): 28

IT **67560-80-9P 67560-82-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methanolysis of)

IT **67560-80-9P 67560-82-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methanolysis of)

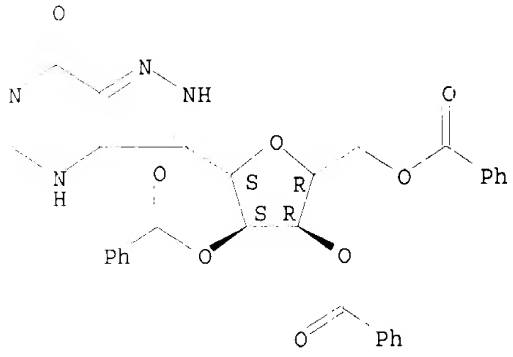
RN 67560-80-9 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



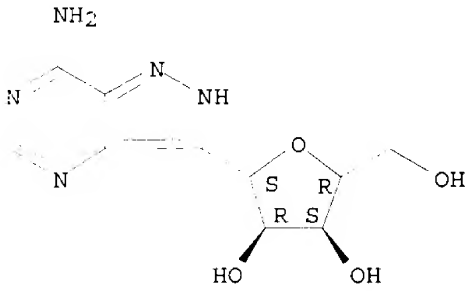
RN 67560-82-1 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:510233 HCAPLUS
DOCUMENT NUMBER: 89:110233
TITLE: Dynamics of tautomerization of formycin
AUTHOR(S): Cole, Francis X.; Schimmel, Paul R.
CORPORATE SOURCE: Dep. Biol., Massachusetts Inst. Technol., Cambridge, Mass., USA
SOURCE: J. Am. Chem. Soc. (1978), 100(12), 3957-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dynamics of tautomerization of formycin A was investigated by the temp.-jump method. The tautomerization between 1-H- and 2-H-formycin was followed spectrophotometrically. In unbuffered solns., the tautomerization is characterized by a single relaxation process with a time const. of around 10-4 sec at 25.degree.. The relaxation time is pH dependent, being faster at acid pH values. The rate of tautomerization of neutral formycin is 3.4 .times. 103 sec-1 (25.degree.) and over 10-fold more rapid for the protonated form. Basic species such as unprotonated imidazole greatly accelerate the rate of tautomerization. The rate detg. step in tautomerization is abstraction by a basic species of a proton from N-1 (or N-2) in the pyrazole part of the ring; the transient intermediate then quickly adds back a proton from the solvent or a protonated base.
CC 23-7 (Carbohydrates)
Section cross-reference(s): 22, 28
IT **57101-52-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by tautomerization)
IT **57101-52-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by tautomerization)
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:468560 HCAPLUS
DOCUMENT NUMBER: 87:68560
TITLE: Fluorescent derivatives of nucleosides
AUTHOR(S): Chung, Hsiao L.; Zemlicka, Jiri
CORPORATE SOURCE: Michigan Cancer Found., Detroit, Mich., USA
SOURCE: J. Heterocycl. Chem. (1977), 14(1), 135-8

CODEN: JHTCAD
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In this abstract, R1 = .beta.-D-ribofuranosyl. The fluorescence specta of anhydro- (I, II and III) and methyleneribonuclosides (IV, V, VI (Q = N, R = H, Br; Q = CH, R = H), and VII were related to the known fluorescent formycin. The aminomethylene group in IV-VII leads to fluorescence but causes bathochromic shifts. I and II fluoresce more strongly than formycin, and show the bathochromic shift.

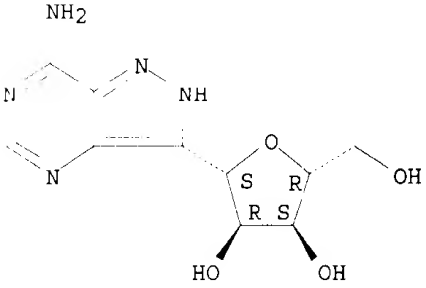
CC 33-7 (Carbohydrates)
Section cross-reference(s): 22, 28

IT 17331-14-5 17331-15-6 17331-16-7 **57101-52-7** 57553-78-3
57573-29-2 57573-30-5 57881-18-2 57881-19-3 **63347-44-4**
63358-78-1
RL: PRP (Properties)
(fluorescence spectrum of)

IT **57101-52-7 63347-44-4 63358-78-1**
RL: PRP (Properties)
(fluorescence spectrum of)

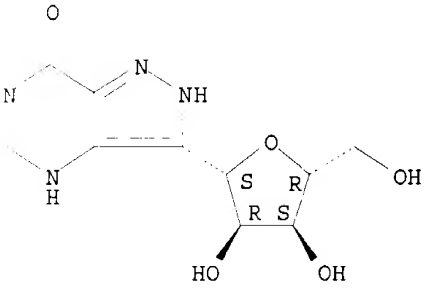
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



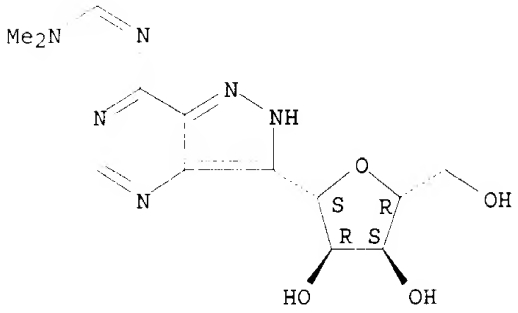
RN 63347-44-4 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



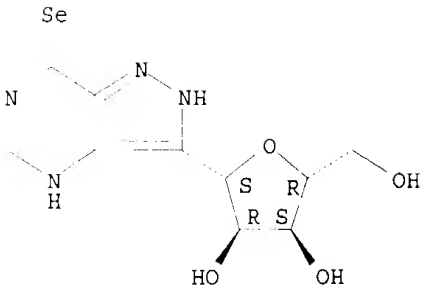
RN 63358-78-1 HCAPLUS
CN Methanimidamide, N,N-dimethyl-N'-(3-.beta.-D-ribofuranosyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L5 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:497797 HCAPLUS
DOCUMENT NUMBER: 83:97797
TITLE: Novel synthesis of 6-seleno-substituted nucleosides, nucleotides, and cyclic nucleotides
AUTHOR(S): Shiue, Chyng-Yann; Chu, Shih-Hsi
CORPORATE SOURCE: Div. Biol. Med. Sci., Brown Univ., Providence, R. I., USA
SOURCE: J. Chem. Soc., Chem. Commun. (1975), (9), 319-20
CODEN: JCCCAT
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Treatment of the amino heterocycles I (X = CH, X1 = N, R = R1 = H, R2 = beta.-D-ribofuranosyl, 3',4'-cyclic phosphoribosyl, arabinofuranosyl; X = CH, X1 = N, R2 = 3',5'-cyclic phosphoribosyl, 5'-phosphoribosyl; X = NH, X1 = C, R = R1 = H, R2 = .beta.-D-ribofuranosyl) with excess H2Se in pyridine-H2O in a sealed tube at 65.degree. gave 21-75% of the title compds. II. Thus, treatment of I (X = CH, X1 = N, R = R1 = H, R2 = .beta.-D-ribofuranosyl) for 5 days gave 56% of the corresponding Se compd.
CC 33-7 (Carbohydrates)
IT 29411-74-3P 40093-99-0P 56477-08-8P 56477-11-3P 56477-14-6P 56477-16-8P **57101-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 58-61-7, reactions 60-92-4 2096-10-8 5536-17-4 10254-91-8 50884-82-7 **57101-52-7**
RL: RCT (Reactant)
(substitution reaction with hydrogen selenide)
IT **57101-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 57101-53-8 HCAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidine-7-selone, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **57101-52-7**
RL: RCT (Reactant)
(substitution reaction with hydrogen selenide)
RN 57101-52-7 HCAPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.